ISSN: 2456-6438

jprmpceditor@scischolars.com Online Publication Date: October 21, 2017 Volume 2, No. 1

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Journal of Progressive Research in Modern Physics and Chemistry

www.scischolars.com

Diffraction of de Broglie Waves

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Abstract

Bohmian mechanics considering particles as de Broglie sources of phase which propagates according to classical electrodynamics affords a methodology for evaluating the diffraction of individual particles. Treating the phasing as optical waves allows for reflections at potential energy barriers by which the phase information of an individual particle can return to direct the motion of the particle. Using this approach, crystallographic diffraction is shown to exemplify the behavior of a particle in a box, and the predictions for single and double slit diffraction also are consistent with optical and particle experiments.

Keywords: de Broglie phase waves; matter diffraction.

1. Introduction

A preceding article [1] used the concept of de Broglie waves to describe the behavior of a particle in an infinite square wave potential (a particle in a box). Our approach is based on the concept that particles of mass m_0 possess phase properties with periodicity ω_0 determined by their energy

$$\omega_0 = \frac{m_0 c^2}{\hbar} \tag{1}$$

Where c is the speed of light and $\hbar$ is Planck's constant using units of radians. For a moving source, the frequency will decrease to $\omega\gamma$ due to relativistic effects, where

$$\gamma \equiv \left(1 - \frac{v^2}{c^2}\right)^{1/2} \tag{2}$$

It was assumed that phase information is transmitted in waves which follow classical optical principles [2], including special relativity, phase changes upon reflection, and interference effects, and that optimum particle trajectories occur for paths in which the phases are coherent. The energies and nodal structure of the excited states obtained by this treatment match the results obtained from the Schrödinger equation for an individual particle in a box.

Here we extend this approach to particle diffraction, including crystallographic diffraction, which affords the Bragg relationship [3], and single and double slit experiments. The results are consistent with observation and optical phenomena [4].

2. Discussion

2.1. Particles translating in a one-dimensional box.

A particle in a one-dimensional horizontal box will develop a momentum perpendicular to the walls. This was proposed to occur for a single particle because the particle serves as a source of phase waves which can reflect from the boundaries [1]. Waves which are reflected twice (and by an even-integer number of times) were shown to determine the momentum of the particle, and single (and odd-integer number) of reflections determine the placement of nodes in the excited states by treating the interference patterns which are established. The situation will be analogous for a particle with a uniform component of velocity parallel to the walls (Figure 1), since this motion can develop by a vertical motion of the observer which should not disturb the system.

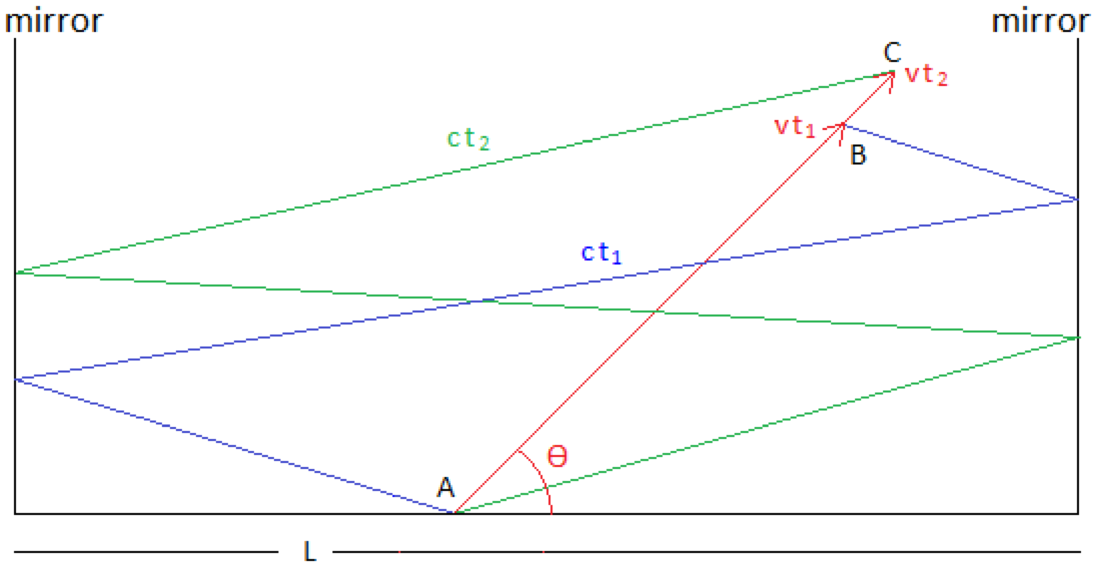

Figure 1. Optical paths for forward (green) and reverse (blue) double reflections returning to a traveling source.

A particle with velocity v emitting at point A will advance a distance vt_1 in the time t_1 for the reverse-emitted reflection (blue), traveling at the speed c, to traverse the distance ct_1 and return at point B. In this time, the emission traverses the vertical distance ($vt_1 \sin\theta$) and the horizontal distance ($2L - vt_1 \cos\theta$). The time to return to the source is

$$\begin{aligned} c^2t_1^2 &= 4L^2 - 4Lvt_1\cos\theta + v^2t_1^2\cos^2\theta + v^2t_1^2\sin^2\theta \\ t_1 &= -2Lv\cos\theta / c^2\gamma^2 + 2L\left[1-(v^2/c^2)+(v^2\cos^2\theta)/c^2\right]^{1/2} / c\gamma^2 \end{aligned} \tag{3}$$

The positive root must be used in Equation 3 for $t_1 > 0$. The situation is similar for the forward-emitted reflection (green), which will return in the longer time t_2.

$$\begin{aligned} c^2t_2^2 &= 4L^2 + 4Lvt_2\cos\theta + v^2t_2^2\cos^2\theta + v^2t_2^2\sin^2\theta \\ t_2 &= 2Lv\cos\theta / c^2\gamma^2 + 2L\left[1-(v^2/c^2)+(v^2\cos^2\theta)/c^2\right]^{1/2} / c\gamma^2 \end{aligned} \tag{4}$$

and the positive root again must be chosen. The root terms (actually their reciprocal) represent the relativistic spatial contraction in the direction of the walls of the box. The difference of these times is

$$\Delta t \equiv t_2 - t_1 = (4Lv\cos\theta)/c^2\gamma^2 \tag{5}$$

This corresponds to the value obtained previously for motion perpendicular to the walls of the box [1] for which $\theta = 0$. For one period

$$\Delta t = 2\pi / \gamma\omega_0 \tag{6}$$

In order to maintain coherence when they return to the source, the phase shift of π for each reflection at the 'hard' barriers restores the original phase relationship between the source and the double reflections, so that the difference in times must be an even integer number ($2l$) of periods [1] $\tau = 2\pi/\gamma\omega_0$ where $l = 1,2,3\ldots$ Then

$$\begin{aligned} \Delta t &= (2l)2\pi/\omega_0\gamma = 4\pi l\hbar / m_0c^2\gamma = (4Lv\cos\theta)/c^2\gamma^2 \\ 2L &= lh\gamma / m_0 v\cos\theta = lh / p_\perp \end{aligned} \tag{7}$$

noting that the total velocity determines the factor γ, which can be neglected for small velocities, whereas $p_\perp = (m_0 v\cos\theta)/\gamma$ is the component of momentum perpendicular to the walls.

2.2. Bragg Diffraction.

A crystal with regular spacing d between atoms or molecules in the crystal would serve as a mirror to (partly) reflect the field of a source traveling within the interstitial space (Figure 2).

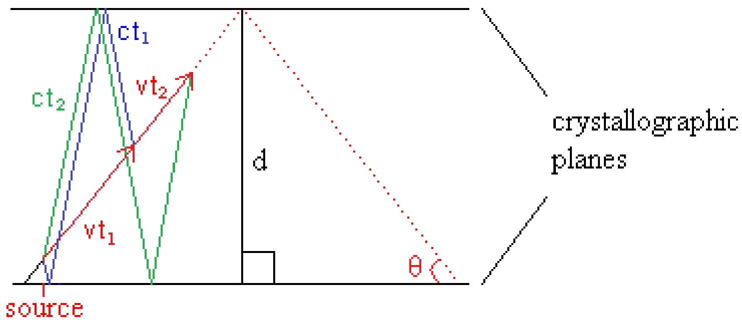

Figure 2. Optical paths for forward and reverse double reflections returning to a source.

Assuming a phase change upon reflection of π, for an incident angle θ, the source will travel in phase with the double reflections from the crystallographic planes for the condition in Equation 7 with $L = d$ and using the complementary angle

$$\begin{aligned} \Delta t &= 2d(v\sin\theta)/c^2\gamma^2 \\ 2\pi l\hbar/mc^2\gamma &= (2dv\sin\theta)/c^2\gamma^2 \\ 2d\sin\theta &= lh/p \end{aligned} \tag{8}$$

This corresponds to Bragg's law [3] for a particle with the de Broglie wavelength $\lambda_{dB} = h/p$:

$$l\lambda_{dB} = 2d\sin\theta \tag{9}$$

2.3. Edge Diffraction.

A source passing an edge will diffract due to reflection from the edge. Since there is a single barrier, it is appropriate to examine the singly-reflected wave returning to the source from the barrier (Figure 3, left). The phase change of π which occurs upon a single reflection needs to be considered. In this case, the number n of intervening periods τ must assume a half-integer value for the reflection to return in phase with the source, so that the time for return would correspond to (n + ½) τ.

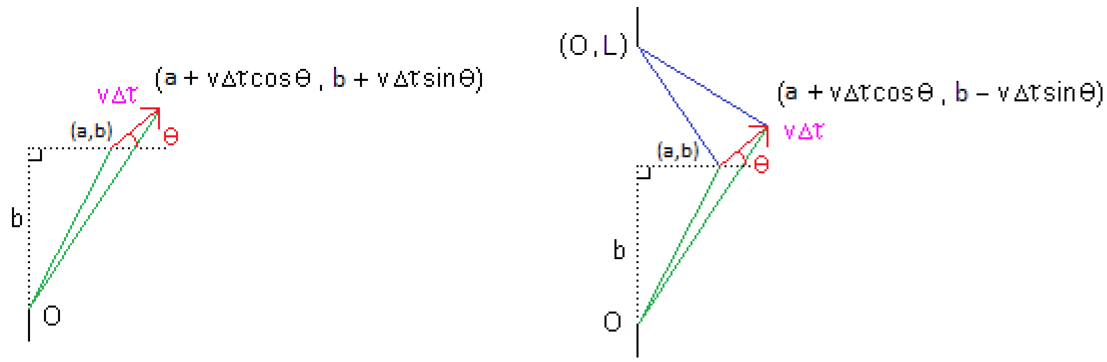

Figure 3. Optical path for single reflection from an edge (left) and from two edges (right) returning to a source.

For an initial position (a, b), the final position after travel of a distance $v\tau$ would be (a + $v\tau\cos\theta$, b + $v\tau\sin\theta$). Then a wave reflecting from an edge at the origin would travel

$$c\tau = \left(a^2 + b^2\right)^{1/2} + \left[(a + v\tau\cos\theta)^2 + (b + v\tau\sin\theta)^2\right]^{1/2} \tag{10}$$

Solving for the angle terms using the quadratic equation affords after some manipulation

$$a\cos\theta + b\sin\theta = \gamma^2 c^2\tau/2v + c\left(a^2 + b^2\right)^{1/2}/v \tag{11}$$

choosing the + root for a nonnegative total path length.

2.4.Single Slit Fraunhofer Diffraction

The situation of a source emerging from a slit resembles edge diffraction, only now there are two edges separated by a distance *L* which reflect (Figure 3, right). Reflection from the lower edge at the origin (*O*) affords the expression derived for diffraction from one edge (Equation 11). Diffraction from the upper edge is obtained by the substitutions

$$\begin{aligned} b &\to b' = L - b \\ \theta &\to \theta' = -\theta \\ \tau &\to \tau' \end{aligned} \tag{12}$$

Taking the difference for a common distance *a* behind the aperture in Figure 3 (right)

$$a\cos\theta + b\sin\theta - [a\cos\theta - b'\sin\theta] = \gamma^2 c^2 \tau / 2v + c\left(a^2 + b^2\right)^{1/2} / v - \left[\gamma^2 c^2 \tau' / 2v + c\left(a^2 + b'^2\right)^{1/2} / v\right] \tag{13}$$

$$L\sin\theta = \gamma^2 \frac{c^2}{v}\frac{\tau - \tau'}{2} + \frac{c}{v}\left[\left(a^2 + b^2\right)^{1/2} - \frac{c}{v}\left[a^2 + (L-b)^2\right]^{1/2}\right]$$

The difference in times $\Delta t = t - t'$ must correspond to an odd-integer number $(2l + 1)$ of periods due to the phase shift of π for each single reflection. For example, for a particle centered in the slit, reflection from one edge might occur one-half wavelength sooner and from the other one-half wavelength later, etc. Using the de Broglie relation

$$2L\sin\theta = (2l+1)\lambda_{dB} + \frac{c}{v}\left[\left(a^2 + b^2\right)^{1/2} - \left[a^2 + (L-b)^2\right]^{1/2}\right] \tag{14}$$

As the particle moves away from the slit, $a >> L$ so b, $L-b \le L << a$ can be neglected

$$L\sin\theta \approx (l + 1/2)\lambda_{dB} \tag{15}$$

so that maxima would be located close to half-integer wavelengths and minima near integer multiples of the wavelength.

The condition for optical minima in single-slit diffraction is

$$L\sin\theta = l\lambda \tag{16}$$

in the Fruanhofer limit, but the condition for maxima is more complicated as the intensity has a sinc dependence. However, these lie close to half-integer values of λ [4], consistent with Equation 15.

2.5. Double-Slit Diffraction

Diffraction also is observed when waves pass through two closely spaced slits. For a system with two narrow slits of width *L* separated by a distance *D*, imagine the edges of the slits to be slightly curved as shown in Figure 4. Then a source emerging from one of the slits would experience three reflected fields: two from the edges of the slit from which it emerges (the bottom slit in the diagram) and one from the far edge of the second slit (the top slit in Figure 4). Considering the origin to be at the lower edge of the lower slit, these reflections would occur at positions (0, 0), (0, L), and (0, L+D). The fourth edge at the lower edge of the top slit (red dashed line at 0, D) would not be reflective for the source.

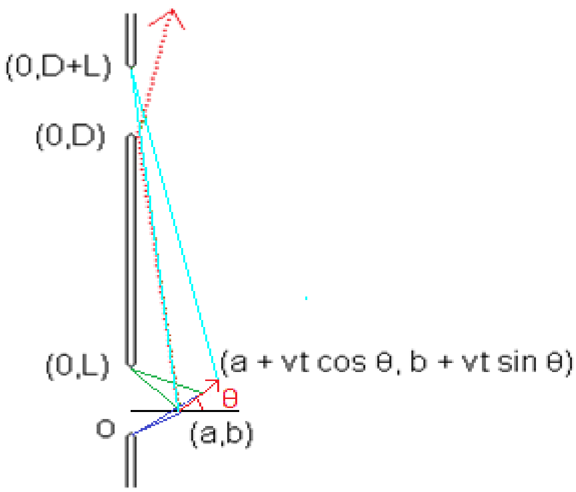

Figure 4. Optical paths for single reflections from the edges of two slits returning to a source.

The three distances traveled by the field from and back to the source then would correspond to three times (t_i) such that

$$\begin{aligned} ct_1 &= [a^2 + b^2]^{1/2} + [(a + vt_1 \cos\theta)^2 + (b + vt_1 \sin\theta)^2]^{1/2} \\ ct_2 &= [a^2 + (L-b)^2]^{1/2} + [(a + vt_2 \cos\theta)^2 + (L - b - vt_2 \sin\theta)^2]^{1/2} \\ ct_3 &= [a^2 + (D+L-b)^2]^{1/2} + [(a + vt_3 \cos\theta)^2 + (D + L - b - vt_3 \sin\theta)^2]^{1/2} \end{aligned} \tag{17}$$

The first two equations are the same as found in single slit diffraction (Equation 13) with $\tau = t_1$ and $\tau' = t_2$ where the difference in times $t_1 - t_2$ must be an odd integer, corresponding to half-integer values of the period τ. The third equation affords

$$\begin{aligned} c^2 t_3^2 &= a^2 + (D+L-b)^2 + (a + vt_3 \cos\theta)^2 + (D + L - b - vt_3 \sin\theta)^2 + \\ &2[a^2 + (D+L-b)^2]^{1/2}[(a + vt_3 \cos\theta)^2 + (D + L - b - vt_3 \sin\theta)^2]^{1/2} \end{aligned} \tag{18}$$

Solving for the angle terms

$$a\cos\theta - (D+L-b)\sin\theta = \gamma^2 c^2 t_3 / 2v \pm c\left[a^2 + (D+L-b)^2\right]^{1/2} / v \tag{19}$$

as expected. Since reflections from the top edge of the bottom slit at (0, L) will introduce a phase shift of one-half wavelength,

$$a\cos\theta - (L-b)\sin\theta = \gamma^2 c^2 t_2 / 2v \pm c\left[a^2 + (L-b)^2\right]^{1/2} / v \tag{20}$$

and the phase shift at the edge (0, D+L) also would be one-half wavelength, the additional distance the field travels to reach the edge at (0, D+L) relative to (0, L) must correspond to an (even) integer number of periods ($n_3 - n_2 = 2l'$)

$$\begin{aligned} &a\cos\theta - (L-b)\sin\theta + D\sin\theta = \gamma^2 c^2 t_2 / 2v \pm c\left[a^2 + (L-b)^2\right]^{1/2} / v + D\sin\theta \\ &= \gamma^2 c^2 t_3 / 2v \pm c\left[a^2 + (D+L-b)^2\right]^{1/2} / v \end{aligned} \tag{21}$$

There is no restriction on the phase from the edge (0, D) since this edge is not reflective (dashed line in Figure 4). Then

$$\begin{aligned} &\gamma^2 c^2 \left(n_2 + \frac{1}{2}\right)\tau / 2v \pm c\left[a^2 + (L-b)^2\right]^{1/2} / v + D\sin\theta \\ &= \gamma^2 c^2 (n_3 + 1/2)\tau / 2v \pm c\left[a^2 + (D+L-b)^2\right]^{1/2} / v \end{aligned} \tag{22}$$

and so here

$$D\sin\theta = \frac{1}{2}\frac{\gamma^2 c^2}{v}(n_3 - n_2)\tau \pm \frac{c}{v}\left\{\left[a^2 + (D+L-b)^2\right]^{1/2} \mp \left[a^2 + (L-b)^2\right]^{1/2}\right\}^{1/2} \tag{23}$$

In the Fraunhofer limit (for a>>D + L), this becomes

$$D\sin\theta \approx \gamma^2 c^2 (n_3 - n_2)\tau / 2v = l'h/p = l'\lambda_{dB} \tag{24}$$

Diffraction of large molecules such as C_{60} passing through a double slit has been observed [5]. Although quantification is complicated by interactions between material particles and the walls of the slits, the most probable result was centered in agreement with Equation 24. Optical diffraction which is well-studied affords maxima in double-slit diffraction near integer values of λ

$$L\sin\theta \approx l\lambda \tag{25}$$

consistent with Equation 24, whereas minima occur at half-integer values [4].

3. Conclusion

The association of particles with phase properties which propagate optically define a de Broglie wave. Interference of these waves when they reflect from physical barriers and coherence phenomena explain optimum particle trajectories for the individual particles serving as the sources of the phase waves. Treatment of crystallographic diffraction as the behavior of a particle in a box affords Bragg's Law for the de Broglie wavelength. Similarly, diffraction by single and double slits is produced by consideration of reflections from the edges of the slits. The preferred particle motion lies along a trajectory where the reflected waves return in phase with the phase of the particle. Some phenomena may be handled more easily in this manner than by other methods such as use of the Schrödinger equation [6], and extension of the concept to varying potentials will be treated subsequently.

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